

# Wang-Landau sampling: a criterion for halting the simulations

A. A. Caparica

*Instituto de Física, Universidade Federal de Goiás. C.P. 131,  
CEP 74001-970, Goiânia, GO, Brazil*

In this work we propose a criterion to finish the simulations of the Wang-Landau sampling. Instead of determining a final modification factor for all simulations and every lattice sizes, we investigate the behavior of the temperature of the peak of the specific heat during the simulations and finish them when this value varies below a given limit. As a result, different runs stop at different final modification factors. We apply this technique to the two-dimensional Ising model and a homopolymer. We verify that for the Ising model the mean order of the final modification factors are roughly the same for all lattice sizes, but for the homopolymer the order of the final modification factors increases with increasing polymer sizes.

Keywords: Wang-Landau sampling; accuracy; efficiency

## I. INTRODUCTION

Wang-Landau sampling (WLS)[1, 2] can be considered a well established Monte Carlo method, since it has been applied efficiently to many systems. Nevertheless the method is still in development and new ideas have contributed to increase the degree of efficiency and accuracy of the algorithm.

The method is based on the fact that if one performs a random walk in energy space with a probability proportional to the reciprocal of the density of states, a flat histogram is generated for the energy distribution. Since the density of states produces huge numbers, instead of estimating  $g(E)$ , the simulation is performed for  $S(E) \equiv \ln g(E)$ . At the beginning we set  $S(E) = 0$  for all energy levels. The random walk in the energy space runs through all energy levels from  $E_{min}$  to  $E_{max}$  with a probability  $p(E \rightarrow E') = \min(\exp[S(E) - S(E')], 1)$ , where  $E$  and  $E'$  are the energies of the current and the new possible configurations. Whenever a configuration is accepted we update  $H(E') \rightarrow H(E') + 1$  and  $S(E') \rightarrow S(E') + F_i$ , where  $F_i = \ln f_i$ ,  $f_0 \equiv e = 2.71828...$  and  $f_{i+1} = \sqrt{f_i}$  ( $f_i$  is the so-called modification factor). The flatness of the histogram is checked after a number of Monte Carlo (MC) steps and usually the histogram is considered flat if  $H(E) > 0.8\langle H \rangle$ , for all energies, where  $\langle H \rangle$  is an average over energies. If the flatness condition is fulfilled we update the modification factor to a finer one and reset the histogram  $H(E) = 0$ . The original version of WLS prescribes that simulations should be in general halted when  $f \sim 1 + 10^{-8}$ . Having in hand the density of states, one can calculate the canonical average of any thermodynamic variable as

$$\langle X \rangle_T = \frac{\sum_E \langle X \rangle_E g(E) e^{-\beta E}}{\sum_E g(E) e^{-\beta E}}, \quad (1)$$

where  $\langle X \rangle_E$  is the microcanonical average accumulated during the simulations.

Recent works [3–5] have demonstrated that (a) instead of updating the density of states after every spin-flip, one

ought to update it after each Monte Carlo sweep[6]; (b) WLS should be carried out only up to  $\ln f = \ln f_{final}$  defined by the canonical averages during the simulations; and (c) the microcanonical averages should not be accumulated before  $\ln f \leq \ln f_{micro}$  defined by the microcanonical averages during the simulation. The adoption of these easily implementable changes leads to more accurate results and saves computational time. They investigated the behavior of the maxima of the specific heat

$$C = \langle (E - \langle E \rangle)^2 \rangle / T^2 \quad (2)$$

and the susceptibility

$$\chi = L^2 \langle (m - \langle m \rangle)^2 \rangle / T, \quad (3)$$

where  $E$  is the energy of the configurations and  $m$  is the corresponding magnetization per spin, during the WLS for the Ising model on a square lattice. They observed (as in [8–11]) that a considerable part of the conventional Wang-Landau simulation is not very useful because the error saturates. In order to define  $f_{final}$  to a given model one should take a representative size ( $L = 32$  for the 2D Ising model and  $N = 50$  for the homopolymer) and find out when the corresponding canonical averages obtained from a few independent runs would come to steady values. In that study they concluded that  $f_{final}$  should be  $f_{13}$  and  $f_{18}$  for the 2D Ising model and the homopolymer, respectively.

In this work we propose a criterion for finishing the simulations which turns the choice of  $f_{final}$  automatic for each independent run. As a result the simulated data become more accurate and one has no need to find out  $f_{final}$  before initiating the simulations.

## II. A CRITERION FOR FINISHING THE SIMULATIONS

From time to time during the WLS the random walker pauses the simulation in order to check the histogram for flatness. The number of MCS between two checks is not

relevant for the final resulting density of states, but it is interesting to relate it to the number of energy levels  $N_E$  of the system. In this work we used  $10N_E$  for the 2D Ising model and  $100N_E$  for the homopolymer.

Applying WLS to the two-dimensional Ising model, beginning from  $f_{11}$ , we calculate the temperature of the peak of the specific heat defined in Eq.(2) using the current  $g(E)$  and from this time on this mean value is updated whenever the histogram is checked for flatness. When the histogram is considered flat, we save the value of the temperature of the peak of the specific heat  $T_c(0)$ . We then update the modification factor  $f_{i+1} = \sqrt{f_i}$  and reset the histogram  $H(E) = 0$ . During the simulations with this new modification factor we continue calculating the temperature of the peak of the specific heat  $T_c(t)$  whenever we check the histogram for flatness and we also calculate the checking parameter

$$\varepsilon = |T_c(t) - T_c(0)|. \quad (4)$$

The idea of the proposed criterion is that if  $\varepsilon$  remains less than a determined value *limit* during this modification factor, then we save the density of states and the micro-canonical averages and stop the simulations. In order to define which would be the ideal value for *limit* we first of all tested the range of variation of the temperatures. Defining  $T_{min}$  and  $T_{max}$  as the minimum and maximum temperatures for  $N_{runs}$  independent runs for a simulation up to  $f_{19}$ , we can define the mean distance between two temperatures as

$$\Delta = (T_{max} - T_{min}) / (N_{runs} - 1). \quad (5)$$

For the Ising model we obtained  $\Delta = 6.0 \times 10^{-4}$  for  $L = 32$  with  $N_{runs} = 24$  and  $\Delta = 3.7 \times 10^{-4}$  for  $L = 80$  with  $N_{runs} = 12$ . Since most of the values of temperature fall close to the center of the range, *limit* should be at least of the order of  $2.0 \times 10^{-4}$ . Nevertheless, as we show in Fig. 1,

$$limit = 10^{-4} \quad (6)$$

is a more stringent, but a safer parameter. Top of Fig. 1 shows the evolution of the temperature of the peak of the specific heat beginning from  $f_{11}$  calculated for  $L = 80$  as a function of the Monte Carlo sweeps[6] using the 80% flatness criterion. The dots show where the modification factor was updated. The lower panel shows the evolution of the checking parameter  $\varepsilon$  during the same simulation. In this example one can see that if  $limit = 2 \times 10^{-4}$  was adopted the simulation would be finished at  $f_{14}$ , before the effective stabilization of the output. Using  $limit = 10^{-4}$  the simulation proceeds up to  $f_{16}$ . The dotted line shows what would be the results if the simulation would be continued up to  $f_{19}$ .

This criterion for finishing the WLS has two main advantages. First of all it is not necessary to determine  $f_{final}$  for a representative size, as prescribed in reference [3] since it is defined automatically for each independent run. The second convenience is that different

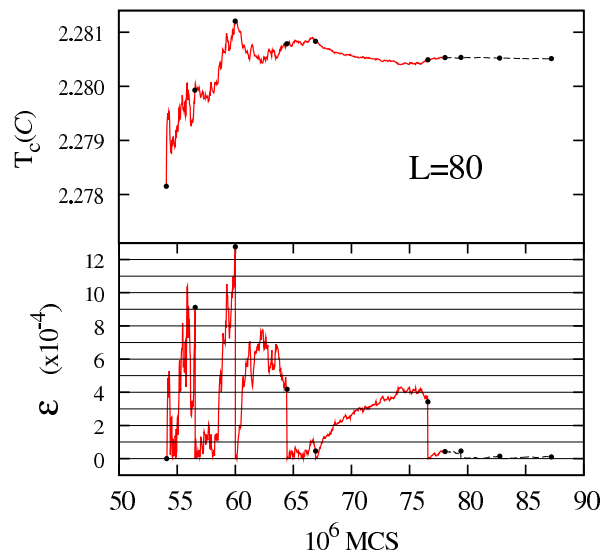


FIG. 1. (color online). Upper panel: Evolution of the temperature of the extremum of the specific heat during the WLS, beginning from  $f_{11}$  for a single run. The dots show where the modification factor was updated. Lower panel: Evolution of the checking parameter  $\varepsilon$  during the same simulation.

runs can proceed up to different final modification factors, depending on the evolution of the simulation.

### III. RESULTS

#### A. 2D Ising model

In order to test the proposed criterion, we performed Wang-Landau simulations of the two-dimensional Ising model with  $L = 32, 36, 40, 44, 48, 52, 56, 64, 72$ , and  $80$ , taking  $N = 24, 24, 20, 20, 20, 16, 16, 16, 12$ , and  $12$  independent runs for each size, respectively, adopting the 80% and the 90% flatness criteria.

$L$	$f_{final}$	
	80%	90%
32	15.67(21)	16.29(11)
36	15.25(14)	16.71(15)
40	15.55(18)	16.45(18)
44	15.55(23)	16.60(17)
48	15.50(15)	16.35(17)
52	15.06(17)	16.25(19)
56	15.31(22)	16.25(23)
64	15.44(22)	16.33(22)
80	15.08(29)	16.92(26)

TABLE I. Mean order of the final modification factor for each simulated size of the 2D Ising model using the 80% and the 90% flatness criterions.

As we pointed out before, different independent runs may finish at different final modification factors. For  $L = 32$  and 80% of flatness  $f_{final}$  ranges from  $f_{14}$  to  $f_{18}$ , and using 90%, from  $f_{15}$  to  $f_{17}$ . For  $L = 80$  we obtained  $f_{14}$ - $f_{17}$  and  $f_{15}$ - $f_{18}$ , respectively.

In Table I we show the mean order of the final modification factors for each lattice size of the simulation. One can see that they are roughly size independent and slightly more stringent than the modification factor  $f_{13}$  prescribed in Ref.[3].

According to finite-size scaling theory [12–14] from the definition of the free energy one can obtain the zero field scaling expressions for the magnetization and the susceptibility, respectively by

$$m \approx L^{-\beta/\nu} \mathcal{M}(tL^{1/\nu}), \quad (7)$$

$$\chi \approx L^{\gamma/\nu} \mathcal{X}(tL^{1/\nu}). \quad (8)$$

We see that the locations of the maxima of these functions scale asymptotically as

$$T_c(L) \approx T_c + a_q L^{-1/\nu}, \quad (9)$$

where  $a_q$  is a quantity-dependent constant, allowing then the determination of  $T_c$ .

Using these scaling functions and assuming  $\nu = 1$ , we estimated the critical temperature and the critical exponents  $\beta$  and  $\gamma$ .

Case	$T_c$	$\beta$	$\gamma$
Exact	2.2691853...	0.125	1.75
Ref.[3]			
80%	2.26934(23)	0.1270(16)	1.7631(27)
90%	2.26916(12)	0.12494(68)	1.7555(32)
Present work			
80%	2.26894(25)	0.1239(13)	1.7562(33)
90%	2.269006(77)	0.12464(45)	1.7572(21)

TABLE II. Finite size scaling results for the critical temperature and the critical exponents  $\beta$  and  $\gamma$ .

In Table II we show our results for the critical temperature and the exponents  $\beta$  and  $\gamma$  and compare them with the exact values and those of Ref.[3]. One can see that the accuracies for the 90% flatness criterion are roughly of the same order in both works, but for the 80% flatness case the adoption of the criterion for finishing the simulations proposed in this paper has lead to improved results. This improvement is welcome because the 90% flatness criterion is in general difficult to apply to other systems[15–18], resulting sometimes in non-convergence or even more inaccurate values.

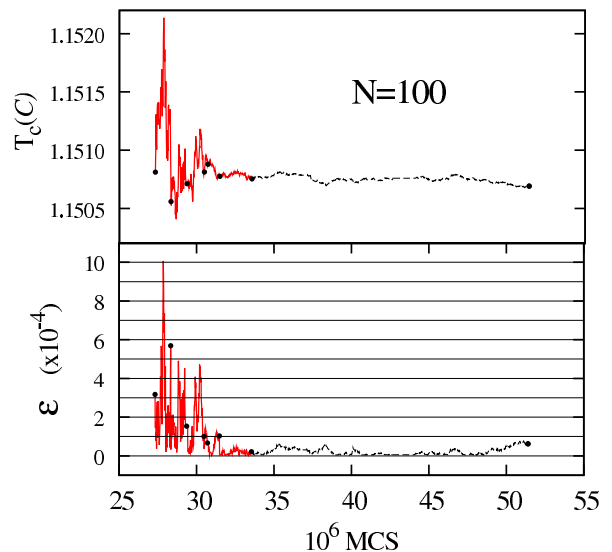


FIG. 2. (color online). Upper panel: Evolution of the temperature of the extremum of the specific heat of the self-avoiding homopolymer of  $L = 100$  during the WLS, beginning from  $f_{16}$  for a single run. The dots show where the modification factor was updated. Lower panel: Evolution of the checking parameter  $\epsilon$  during the same simulation.

## B. Homopolymer

$N$	$f_{final}$	$N$	$f_{final}$
	80%		80%
40	18.70(30)	110	22.30(70)
50	19.60(40)	110	23.10(69)
60	20.00(49)	120	23.50(92)
70	21.50(40)	130	25.00(30)
80	21.50(45)	140	25.30(45)
90	21.22(52)	150	24.30(45)

TABLE III. Mean order of the final modification factor for each simulated size of homopolymers using the 80% flatness criterion.

As a new application of the criterion, we consider a homopolymer consisting of  $N$  monomers which may assume any self avoiding walk (SAW) configuration on a two-dimensional lattice. Assuming that the polymer is in a bad solvent, there is an effective monomer-monomer attraction in addition to the self-avoidance constraint representing excluded volume. For every pair of non-bonded nearest-neighbor monomers the energy of the polymer is reduced by  $\epsilon$ . The Hamiltonian for the model can be written as

$$\mathcal{H} = -\epsilon \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad (10)$$

where  $\sigma = 1(0)$  if the site  $i$  is occupied(vacant), and the sum is over nearest-neighbor pairs[19]. (The sum is understood to exclude pairs of bonded segments along the chain.) We used the so-called reptation or “*slithering snake*” move which consists of randomly adding a monomer from one end of the chain and removing a monomer from the other end, maintaining the size of the polymer constant. We define one Monte Carlo step as  $N$  attempted moves.

We performed simulations for polymers of sizes  $N = 40, 50, 60, 70, \dots, 150$  taking 10 independent runs for each size and finishing the process when the condition

$$|T_c(t) - T_c(0)| < 10^{-4} \quad (11)$$

was satisfied in the course of the whole simulation of a modification factor, where again,  $T_c(0)$  is the last temperature of the peak of the specific heat in the previous modification factor.

In Fig.2 we show the evolution of the temperature of the extremum of the specific heat of a polymer of  $N = 100$ , beginning from  $f_{16}$ . In the lower panel the checking parameter  $\varepsilon$  of the same simulation is displayed. The dotted lines are the continuation of the simulation for one extra modification factor. Now  $f_{final}$  varies from  $f_{17}$  to  $f_{20}$  for  $L = 40$  and from  $f_{22}$  to  $f_{26}$  for  $L = 150$ , for example.

In Table III we show the mean order of the final modification factor for each polymer size. One can see that unlike the two-dimensional Ising model, in this case the order of the final modification factor increases with increasing polymer sizes. Adopting the proposed criterion for halting the simulations guarantees that each particular run proceeds up to the real stabilization of the results.

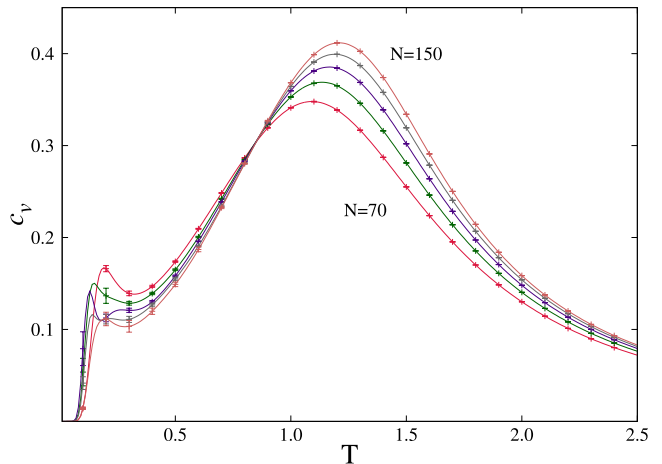


FIG. 3. (color online). Specific heat per monomer as a function of temperature for  $N = 70, 90, 110, 130$  and  $150$ , which yield ground state energies  $E_g = -54, -72, -90, -108$  and  $-126$ , respectively.

In Fig. 3 we show the specific heat per monomer of the homopolymer for several chain sizes. The simulations were started from constructed ground state configurations[24].

In both examples of models discussed here we have obtained good results by adopting  $limit = 10^{-4}$ , but when applying the method to more elaborate models, such as the HP model of protein folding[20, 21] or continuous (off-lattice) models of polymers[22, 23] one should always observe the evolution of the canonical average for each new case, not excluding the possibility of adopting a more stringent parameter, such as  $limit = 5 \times 10^{-5}$ , if the convergence is shown to be more unstable.

#### IV. CONCLUSIONS

We proposed a criterion to finish the simulations of the Wang-Landau sampling. Instead of determining a final modification factor  $f_{final}$  for all simulations and every lattice sizes, the behavior of the temperature of the peak of the specific heat is checked during the simulations and the process is halted when this value varies below a given limit during the whole simulation of a modification factor. As a result, different runs stop at different final modification factors. We applied this technique to the two-dimensional Ising model and a homopolymer and found that for the Ising model the mean final order of the modification factors are roughly the same for all lattice sizes, but for the homopolymer the final order of the modification factor increases with increasing polymer sizes.

#### V. ACKNOWLEDGMENT

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